RJA 1/6/22
JS 12/21/21

Fate Report for Case # P-18-0077

Fate
Summary Statement

Fate Summary Statement: P-18-0077

FATE: Estimations for hydrolysis product N-butylphosphorothioic triamide,
MW = 167, C4H14N3PS
log Kow = 0.44 (M)
log Koc =
1.34 (E)
log Fish BCF = 0.50 (3) (E)
log Fish BAF = 0.03 (1) (E)

FATE: Estimations for hydrolysis product urea-formaldhyde oligomer, MW = 162, C4H10N4O3
log Kow = -4.01 (E)
log Koc = 1.00 (E)
log
Fish BCF = 0.50 (3) (E)
log Fish BAF = -0.05 (1) (E)
PMN
Substance: Solid with MP = Dec. 150 °C (M)
log Kow = 0.60 (M for
mixture)
S = Reacts / 35 mg/L at 25 °C / 37 g/L at 25 °C (M / M for
mixture / E)
Hydrolysis Half-life = hr-da
VP = 3.3E-6 torr at 25
°C (E)
BP = 393 °C (E)
H < 1.00E-8 (E)
POTW removal (%) =
PMN 90 via hydrolysis; then Hyd Pdt NBPT 0-10;
Hyd Pdt
urea-formaldehyde oligomers 75-90 via biodeg and hydrolysis; Hydrolysis (OPPTS 835.2120): t1/2(pH4,7,9):hr/hr-da/da
Time for complete ultimate
aerobic biodeg = Hyd Pdt NBPT > mo;
Hyd Pdt urea-formaldehyde
oligomers wk
Sorption to soils/sediments = Hyd Pdt NBPT low; Hyd Pdt
urea-formaldehyde oligomers low
PBT Potential: PMN P1B1; Hyd Pdt NBPT

P3B1; Hyd Pdt urea-formaldehyde oligomers P1B1
*CEB FATE: Migration to
ground water = Hyd Pdt NBPT rapid;
Hyd Pdt urea-formaldehyde
oligomers slow
Bioconcentration factor to be put into E-FAST: Hyd Pdt
NBPT 3;
Hyd Pdt urea-formaldehyde oligomers 3

PMN Material:

Overall wastewater treatment removal is 90% via rapid hydrolysis (hydrolysis half-life: hours to days).
PMN Material:
Low
Persistence (P1) is based on rapid hydrolysis (hydrolysis half-life: hours to days).
Low Bioaccumulation potential (B1) is based on rapid
hydrolysis (hydrolysis half-life: hours to days).
Hydrolysis Product
(N-butylphosphorothioic triamide):
Overall wastewater treatment
removal is 0-10% via low biodegradability, low sorption and low stripping.

Sorption to sludge is low based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates.
Air Stripping
(Volatilization to air) is negligible based on the estimated
physical-chemical properties from EPISUITE and STPWIN model estimates.

Removal by biodegradation in wastewater treatment is negligible based on BIOWIN model estimates and data from analogous chemicals.
The
aerobic aquatic biodegradation half-life is greater than months based on BIOWIN model estimates and data from analogous chemicals.
The
anaerobic aquatic biodegradation half-life is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life.
Hydrolysis half-life is greater than
months based on measured data (hydrolysis half-life: 92 days at pH 7 and 58 minutes at pH 3).
Sorption to soil and sediment is low based on
the estimated physical-chemical properties from EPISUITE.
Migration
to groundwater is rapid based on the estimated physical-chemical

properties from EPISUITE.
Hydrolysis Product (N-butylphosphorothioic triamide):
High Persistence (P3) is based on the estimated anaerobic biodegradation half-life.
Low Bioaccumulation potential (B1) is based on the BCFBAF model estimates.
Hydrolysis Product (Urea-Formaldehyde oligomer):
Overall wastewater treatment removal is 75-90% via biodegradation and hydrolysis.
Sorption to sludge is low based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates.
Air Stripping (Volatilization to air) is negligible based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates.
Removal by biodegradation in wastewater treatment is moderate based on BIOWIN model estimates.

The aerobic aquatic biodegradation half-life is weeks based on BIOWIN model estimates.
The anaerobic aquatic biodegradation half-life is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life.
Hydrolysis half-life is days based on analogous chemicals and professional judgment.

Sorption to soil and sediment is low based on the estimated physical-chemical properties from EPISUITE.
Migration to groundwater is slow, mitigated by biodegradation and hydrolysis.
Hydrolysis Product (Urea-Formaldehyde oligomer):
Low Persistence (P1) is based on further hydrolysis of the urea-formaldehyde oligomer (hydrolysis half-life: days).
Low Bioaccumulation potential (B1) is based on BCFBAF model estimates.
Bioconcentration/Bioaccumulation factor to be put into E-Fast: 3 (hydrolysis products).

[redacted]

Fate Assessor: Card, Marcella

SMILES:	

Physical Properties

Property	Measured/Calculated Value	EPI
Molecular Form:	C6 H18 N5 O P S	C6 H18 N5 O1 P1 S1 (Parent)
Molecular Wt.:	239.23	239.28
% < 500:		
% < 1000:		

Property	Measured Value	Method	Estimated Value	Method	EPI
Melting Point:			Dec. ca. 150	DSC	85.17
Boiling Point:					392.81
BP Pressure:			@760		@760
Vapor Pressure:			0.000003	EPI, low wt.	3.29e-006
Water Solubility:	0.035000	Exp.	37.1[redacted]	EPI low wt/exp	
Log P:	0.60	Exp.	-1.69		
Log Kow:					-1.69
Log Koc:					1.17
Log BCF:					3.1600
Henry's Law:					1.00e-008

pH:	
pH Comment:	

Fate Analysis

Hydrolysis (t1/2, da):		**Volatilization (t1/2) - River (hr):**	1000.0000	**Volatilization (t1/2) - Lake (da):**	1000.0000
Atm Ox Potential (t1/2)OH (hr):	0.2000	**Atm Ox Potential (t1/2)O3 (hr):**		**Atm Ox Potential (t1/2) Total (hr):**	0.2000

MITI Linear:		**MITI NonLinear:**	
Biodeg Linear:	0.7400	**Biodeg NonLinear:**	0.8100
Biodeg Survey ult:	WK	**Biodeg Survey Prim:**	DA
STP (% removal) Total:	1.8500	**STP (% removal) Biodeg:**	0.0900
STP (% removal) Ads:	1.7500	**STP (% removal) Air:**	0.0000

Rationales

Removal in Wastewater Treatment:	
Atmospheric Oxidation:	
Hydrolysis:	
Photolysis:	
Aerobic Biodegradation:	
Anaerobic Biodegradation:	
Sorption to Soil and Sediment:	
Migration to Groundwater:	
Persistence - Air:	
Persistence - Water:	
Volatilization from Water:	
Soil:	
Sediment:	
Other:	
Standard:	
Bioaccumulation:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	PBT Comments
1	1	2	PMN

Persistence	Bioaccumulation	Toxicity	PBT Comments
3	1	2	Hyd Pdt NBPT
1	1	2	Hyd Pdt urea-formaldehyde oligomers

Exposure-Based Testing

Exposure-Based Testing:	

Fate Ratings
Removal in WWT/POTW (Overall):

Removal in WWT/POTW (Overall):	90;0-10;75-90

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
WWT/POTW Sorption:	;1;1	Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:	;4;4	Extensive	Moderate	Low	Negligible	
Biodegradation Removal:	;4;3	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:		Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	;4;2	<= Days	Weeks	Months	> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	;4;4	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Hydrolysis (t1/2 at pH 7,25C) A:	2-3	<= Minutes	Hours	Days	>= Months	P-NR
		<= Minutes	Hours	Days		

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
Hydrolysis (t1/2 at pH 7,25C) B:					>= Months	
Sorption to Soils/Sediments:	;4;4	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	;4;2	Negligible	Slow	Moderate	Rapid	;Hyd Pdt NBPT rapid; Hyd Pdt urea-formaldehyde oligomers slow
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	

Bio Comments:

Bio Comments: PMN; Hyd Pdt NBPT; Hyd Pdt urea-formaldehyde oligomers. Fate studies are available. Fish log BAF = -0.05 (1). Hydrolysis (OPPTS 835.2120): t1/2(pH4,7,9):hr/hr-da/da. The PMN material hydrolyzes with a half-life of hours to days at pH 7 with one of the hydrolysis products being N-butyl- phosphorothioic triamide, and other hydrolysis products expected to be urea-formaldehyde oligomers; the hydrolysis reaction proceeds more rapidly at pH 4 (hours) and slowly (days) at pH 9. In addition, N-butyl- phosphorothioic triamide, has a hydrolysis half-life of 92 days at pH 7 but 58 minutes at pH 3 and is known to degrade rapidly in acidic soils.

Fate Comments:

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to groundwater is rapid based on the estimated physical-chemical properties from EPISUITE.
Hydrolysis Product (N-butylphosphorothioic
triamide):
High Persistence (P3) is based on the estimated anaerobic biodegradation half-life.
Low Bioaccumulation potential (B1) is
based on the BCFBAF model estimates.
Hydrolysis Product
(Urea-Formaldehyde oligomer):
Overall wastewater treatment removal is
75-90% via biodegradation and hydrolysis.
Sorption to sludge is low
based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates.
Air Stripping (Volatilization to air) is
negligible based on the estimated physical-chemical properties from

EPISUITE and STPWIN model estimates.
Removal by biodegradation in
wastewater treatment is moderate based on BIOWIN model estimates.

The aerobic aquatic biodegradation half-life is weeks based on BIOWIN model estimates.
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Hydrolysis
Product (Urea-Formaldehyde oligomer):
Low Persistence (P1) is based
on further hydrolysis of the urea-formaldehyde oligomer (hydrolysis half-life: days).
Low Bioaccumulation potential (B1) is based on
BCFBAF model estimates.
Bioconcentration/Bioaccumulation factor to be
put into E-Fast: 3 (hydrolysis products).

Comments/Telephone Log

Artifact	Update/Upload Time